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1. Introduction

Because of its diverse applicabilities particularly in fluid flow through porous media (i.e. marine sediments), percolation phenomena have been the subject of active research for a long time [1, 2]. Site and bond percolations are mostly studied, and have been quite successful in understanding the physical and chemical properties of inhomogeneous materials (alloys in particular). In most of the polymeric materials i.e. the gel networks, the basic units/segments that form the incipient infinite network, are chains and loops of various sizes [3]. In order to understand the strength of connectivity at the onset of the infinite network, it would be interesting to study a model of percolating networks with chains and loops of various sizes as basic units. Site and bond percolation mechanisms may not be adequate to describe the conformational properties of such random networks. On the other hand, it is rather difficult to consider both loops and chains of various sizes and distributions, because of limitations on computer memory and time. Therefore, it might be useful to investigate the percolation of chains.

Drory et al. [4] have recently studied the percolation threshold of permeable

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objects of various shapes in continuum space. They found that the percolation threshold depends strongly on the size and shapes (i.e. aspect ratio for elongated boxes, radius for spheres, etc). Here we have investigated the percolation of stiff-chains (sticks or thin rods) of various sizes in a two-dimensional discrete lattice; we also find a strong dependence of the percolation threshold on the chain length. Such studies may be helpful in short fibres epoxy resin composites [5]. A related study on jamming coverage has been recently carried out by Svrakic and Henkel [6] for an irreversible deposition of mixtures of line-segments on a square lattice. We have also observed the jamming coverage to decrease with the chain-length, however, we concentrate here primarily on percolation quantities for monodisperse chains. In the following section we describe the model. In section three the results of the simulation are presented with a summary and discussion in section four.

2. Model

We consider a square lattice, and sticks (i.e. stiff-chains) as the percolating units. In classical percolation theory one studies the statistics of a single percolating site. We wish to study the statistics of percolating chains where a chain is defined as multiple percolating sites connected in a linear fashion. Thus the length of a chain L_c is the number of linearly connected sites on the lattice; $L_c = 1$ corresponds to standard site percolation. For a fixed chain-length L_c, we generate clusters of connected chains in the following way. The decision to place a chain is determined with a probability p with the help of pseudo-random numbers. If the random number is less than or equal to p, then we randomly select one of the four directional orientations. The chain is then placed along the chosen direction if no occupied lattice site is in the way as two chains are not allowed to share a lattice site. If the randomly selected orientational direction fails, then we choose another empty site randomly, and a random orientational direction. Therefore, a chain is not placed if it were to intersect with a previously occupied lattice site. This process of selecting an empty site with probability p, and one of the orientational directions randomly, and attempt to place the chain is repeated again and again, for a fixed concentration of occupied sites. The consequence of this rule is that a jamming concentration limit p_j is reached when it is not possible to place additional chains in the lattice. The jamming coverage is less than one for L_c larger than one. We concentrate here mainly on the percolation quantities, and focus on the cluster size, their number, percolation probability and the second moment of the cluster size distribution. In this study, a cluster is defined by joining the nearest-neighbor occupied sites, thus two neighboring sticks will be part of the same cluster if they are separated by one lattice constant.

3. Results

Simulations are carried out on CONVEX C1XP2 machine with 32 MB of memory. This computer contains a vector processor, yet we were unable to make maximum use due to the lack of vector code in the algorithm. For each probability p, two hundred independent runs are used on a 1000×1000 lattice with various size chains. A typical computation requires two hours of processing time for each set of realizations. Twenty-eight different values of p were used for seven different chain-lengths. About 400 hours of computer time was used in this project.

As we mentioned above, we have analysed percolation probability P_∞, cluster number, and the second moment $S = \langle s^2 \rangle$ of the cluster size distribution. The percolation threshold was determined by finding the peak in the second moment. The result of the percolation threshold versus chain-length is shown in fig. 1. We see that the percolation threshold decreases on increasing the chain-length. When shown on a log–log plot this decay exhibits a exponent power-law dependence i.e. $p_c(L_c) \sim L_c^{-x}$. This exponent x was found using a least-squares technique to be about one half.

The exponent beta is determined by examining the percolation probability data with $P_\infty \sim (p - p_c)^\beta$. Fig. 2 shows this percolation probability i.e. probability that a site is a member of the infinite cluster versus the probability that a site is occupied for various chain-lengths. Again, it can be seen that the percolation threshold decreases with increasing chain-length. It should also be noted that the percolation probability saturates at a value of p less than one. The saturation value of P_∞ is the jamming coverage [6], and it decreases with increasing chain-length as expected.

From the least-square fit of the log–log plot of P_∞ versus $(p - p_c)$ we estimate β. We have evaluated β for various chain-lengths and the results are presented in table 1. Within the range of the deviations, these values for β seem to remain the same for different chain-lengths, and is consistent with the accepted values for site and bond percolation [1].

Variation of the second moment S (i.e. the susceptibility) with concentration p is shown in fig. 3 for various chain-lengths. The concentration where S reaches its maximum value is the percolation threshold. Again, it is clear from the data that the percolation threshold decreases with increasing chain-length. A log–log plot of S versus $(p - p_c)$ gives the exponent γ, $S \sim (p - p_c)^{-\gamma}$. The

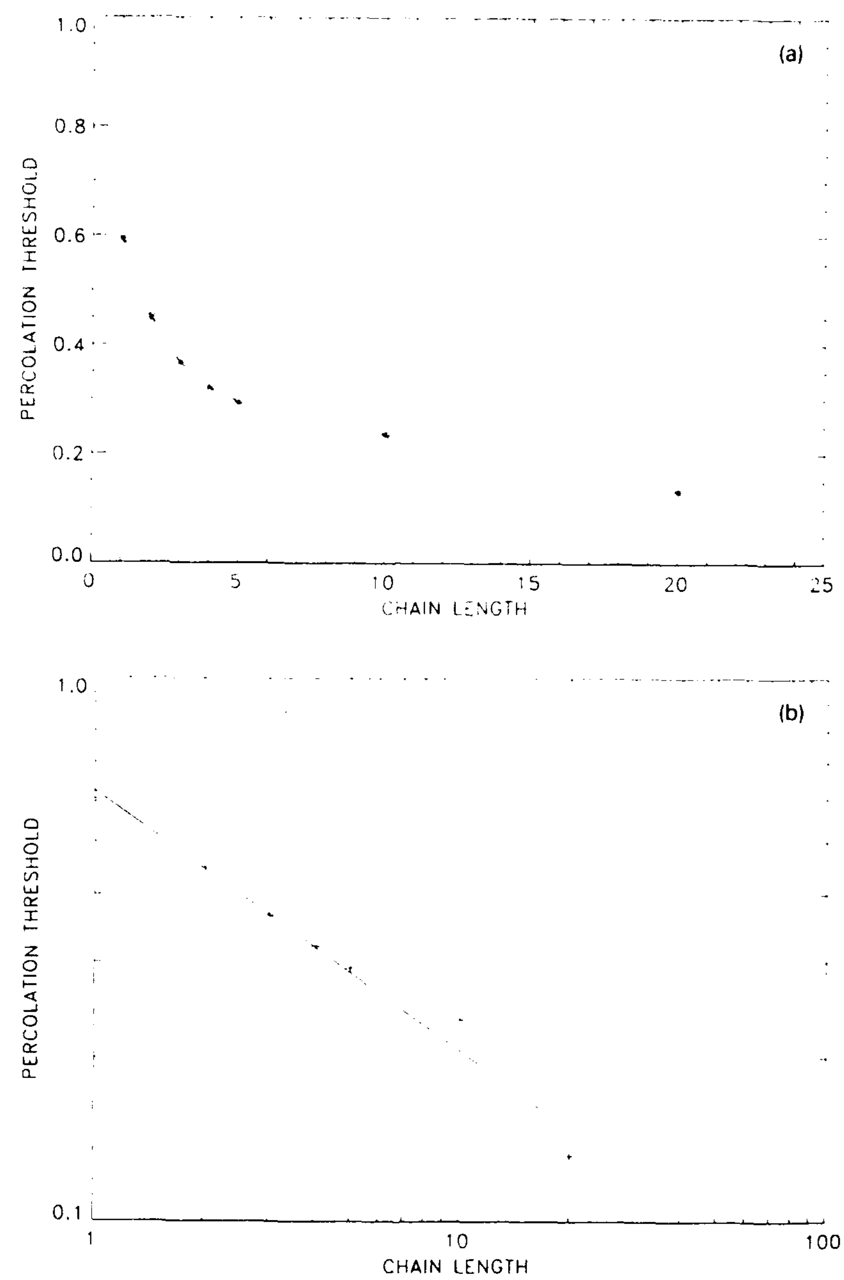

Fig. 1. Percolation threshold p_c versus chain-length (a) linear scale, and (b) log–log scale.

values of γ for various chain-lengths are presented in table I which appears to show no change with chain length (+ and − denote the estimates at p above and below p_c, respectively).

Using the scaling relations [1], other exponents like the correlation length exponent ν can be estimated. The fractal dimensionality D may also be evaluated from $D = d - \beta/\nu$. The computed values for ν and D for various chain-lengths are collected in table 1 for various chain-lengths.

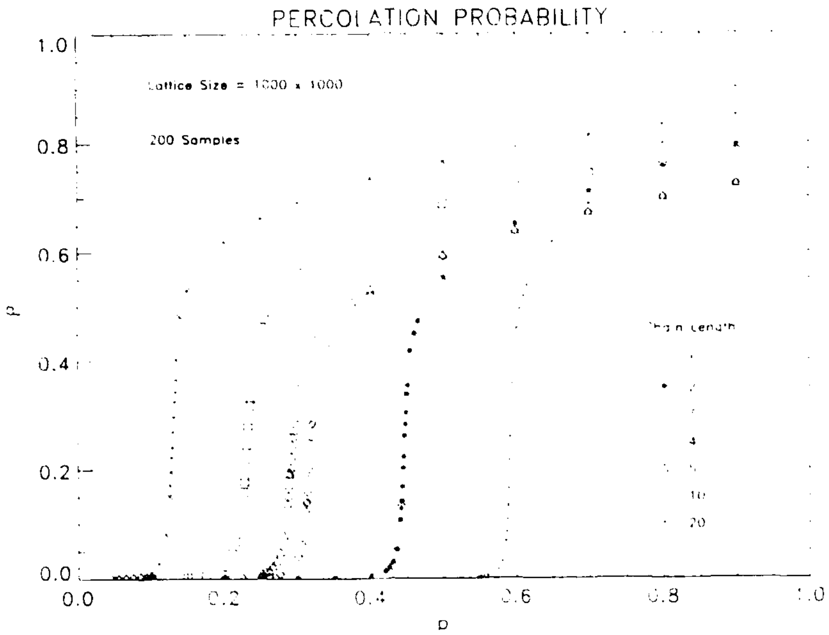

Fig. 2. Percolation probability P versus concentration p of occupied sites. Different symbols represent the different chain-lengths.

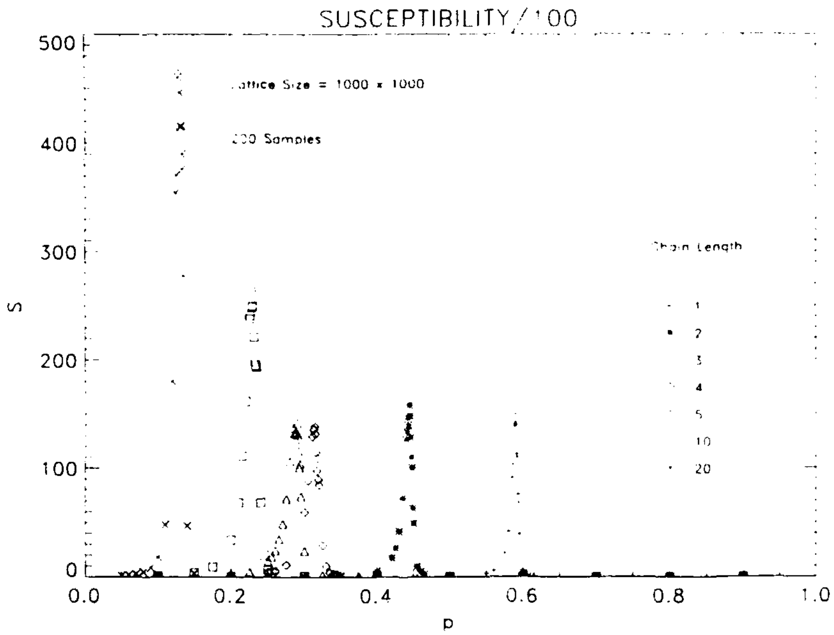

Fig. 3. Variation of the second moment S and p. Different chain-lengths are overlayed using different symbols.

Table 1

L_c	p_c	β	$\gamma(+)$	$\gamma(-)$	ν	D
1	0.593	0.139	2.12	2.07	1.20	1.88
2	0.448	0.137	2.23	1.83	1.25	1.93
3	0.366	0.140	2.27	1.63	1.28	1.91
4	0.321	0.139	2.37	1.45	1.32	1.90
5	0.293	0.143	2.34	1.60	1.31	1.91
10	0.235	0.139	2.40	2.09	1.34	1.90
20	0.132	0.138	2.41	2.46	1.34	1.90

4. Summary

We have presented a computer-simulation study of the percolation of stiff chains/sticks in a two-dimensional lattice. The percolation exponents seem to remain unchanged. The percolation threshold, on the other hand, depends strongly on the chain-length L_c with a power-law $p_c \sim L_c^{-1/2}$. The jamming coverage decreases with the chain-length. We plan to study the percolation of random chains in the near future.

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